Nonlinear energy-loss straggling of protons and antiprotons in an electron gas

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The electronic energy-loss straggling of protons and antiprotons moving at arbitrary nonrelativistic velocities in a homogeneous electron gas are evaluated within a quadratic response theory and the random-phase approximation (RPA). These results show that at low and intermediate velocities quadratic corrections reduce significantly the energy-loss straggling of antiprotons, these corrections being, at low-velocities, more important than in the evaluation of the stopping power.

The energy loss of charged particles has received a great deal of attention for several decades [1–5], since it plays an important role in investigating the elemental composition, depth distribution, and lattice location of implanted atoms in matter. The characterization of the distribution of energy losses suffered by ions in their interaction with matter requires, in the simplest case, two quantities: the stopping power and the energy-loss straggling. Calculations of the energy-loss straggling of charged particles in an electron gas were performed [6], within linear response theory, by treating the screened interaction to lowest order in the projectile charge (Z_1e). This procedure leads results for the stopping power and the energy-loss straggling that are proportional to $Z_1^2e^2$. However, early measurements by Barkas et al. [7] on positive and negative pions, and also subsequent experiments with protons and antiprotons [8], have indicated that these quantities exhibit a dependence on the sign of the projectile charge. This dependence was ascribed to Z_1^3 corrections to the first Born approximation that underlies the linear response theory, assuming that higher odd power corrections were negligible in the velocity regime under study. Very recent measurements [9] of the stopping power for antiprotons in light and heavy targets have shown that the stopping power for antiprotons is reduced, near the stopping maximum, significantly (about 35%) as compared to the corresponding stopping power for protons.

The Z_1^3 correction to the stopping power was first calculated by using classical perturbation theory for a harmonic oscillator [10], and quantal calculations of the Z_1^3 correction to the stopping power of an electron gas have also been performed, in the low [11] and high [12,13] velocity limits. More recently, a quadratic response theory for the interaction of charged particles with an electron gas has been developed [14], in which full account of the Fermi motion of the target is taken into account, and calculations, within this theory, of the stopping power of an electron gas for ions moving with arbitrary nonrelativistic velocities [15] have provided good agreement with measurements of the energy loss of protons and antiprotons in silicon [8]. A calculation of the Z_1^3 correction to the energy-loss straggling and the energy width of the states of ions moving in an electron gas has also been reported, in the low-velocity limit, and it has been demonstrated [14,16] that this correction to the quantities that characterize the distribution of electronic energy losses, i.e., the stopping power, the energy-loss straggling and the energy width coincides, in this limit, with the result of full nonlinear density-functional calculations [17–19], for high electron densities and small projectile charges.

In this paper we investigate, within the full random-phase approximation (RPA), the Z_1^3 correction to the energy-loss straggling of protons and antiprotons moving with arbitrary nonrelativistic velocities in an electron gas. The electron gas model is well-known to account for the contribution to both the stopping power and the energy-loss straggling coming from the interaction of the projectile with valence electrons in metals [20], and the total contribution to these quantities coming from all target electrons has also been computed, on the basis of the electron gas model of the target, by using the so-called local plasma approximation [5]. The results throughout this paper will be expressed in Hartree atomic units, i.e., $\hbar = m = e = 1$.

We consider an ion of charge Z_1 moving with constant velocity $\mathbf{v}$ through an isotropic homogeneous electron gas embedded in a uniformly distributed positive background. The energy-loss straggling per unit path length of the projectile, $\mathrm{d}\Omega^2/\mathrm{d}x$, can be expressed in terms of the probability of transferring momentum $\mathbf{q}$ and energy ω to the electron gas, $P(\mathbf{q},\omega)$, as [20]

$$\frac{\mathrm{d}\Omega^2}{\mathrm{d}x} = \frac{1}{v}\int d\mathbf{q}\int_0^\infty \omega^2 P(\mathbf{q},\omega)\mathrm{d}\omega. \qquad (1)$$

An explicit expression for this probability is given, up to third order in the projectile charge, in Ref. [14], by

following a perturbation-theoretical analysis of the many-body interactions between the moving charge and the electron gas. Using this probability one finds, within the RPA, from Eq.(1):

$$\frac{\mathrm{d}\Omega^2}{\mathrm{d}x} = \left(\frac{\mathrm{d}\Omega^2}{\mathrm{d}x}\right)_L + \left(\frac{\mathrm{d}\Omega^2}{\mathrm{d}x}\right)_Q, \tag{2}$$

where $\left(\mathrm{d}\Omega^2/\mathrm{d}x\right)_L$ and $\left(\mathrm{d}\Omega^2/\mathrm{d}x\right)_Q$ represent contributions to the energy-loss straggling that are proprotional to Z_1^2 and Z_1^3, respectively. $\left(\mathrm{d}\Omega^2/\mathrm{d}x\right)_L$ represents the well-known result one obtains within linear response theory [20]:

$$\left(\frac{\mathrm{d}\Omega^2}{\mathrm{d}x}\right)_L = 2\frac{Z_1^2}{v}\int\frac{\mathrm{d}^3\mathbf{q}}{(2\pi)^3}\omega^2\mathcal{V}_{\mathbf{q}}\mathrm{Im}(-\epsilon_q^{-1})\theta(\omega), \tag{3}$$

and $\left(\mathrm{d}\Omega^2/\mathrm{d}x\right)_Q$ appears as a consequence of the so-called quadratic response of the electron gas:

$$\begin{aligned}\left(\frac{\mathrm{d}\Omega^2}{\mathrm{d}x}\right)_Q &= -4\frac{Z_1^3}{v}\int\frac{\mathrm{d}^3\mathbf{q}}{(2\pi)^3}\omega^2\mathcal{V}_{\mathbf{q}}\theta(\omega)\int\frac{\mathrm{d}^3\mathbf{q}_1}{(2\pi)^3}\mathcal{V}_{\mathbf{q}_1}\\ &\times\mathcal{V}_{\mathbf{q}-\mathbf{q}_1}\left[f_1(q,q_1)+f_2(q,q_1)+f_3(q,q_1)\right],\end{aligned} \tag{4}$$

with

$$f_1(q,q_1) = \mathrm{Im}\epsilon_q^{-1}\mathrm{Re}\epsilon_{q_1}^{-1}\mathrm{Re}\epsilon_{q-q_1}^{-1}\mathrm{Re}M_{q,q_1}^s, \tag{5}$$

$$f_2(q,q_1) = \mathrm{Re}\epsilon_q^{-1}\mathrm{Re}\epsilon_{q_1}^{-1}\mathrm{Re}\epsilon_{q-q_1}^{-1}H_{q,q_1}^s, \tag{6}$$

and

$$f_3(q,q_1) = -2\mathrm{Im}\epsilon_q^{-1}\mathrm{Im}\epsilon_{q_1}^{-1}\mathrm{Re}\epsilon_{q-q_1}^{-1}H_{q,q_1}^s. \tag{7}$$

Here, $q=(\mathbf{q},\omega)$, $q_1=(\mathbf{q}_1,\omega_1)$, $\mathcal{V}_{\mathbf{q}}$ is the Fourier transformation of the electron-electron bare Coulomb interaction,

$$\mathcal{V}_{\mathbf{q}} = \frac{4\pi}{\mathbf{q}^2}, \tag{8}$$

ϵ_q is the longitudinal dielectric function of the medium, M_{q,q_1}^s represents the quadratic response function, H_{q,q_1}^s is related to the imaginary part of M_{q,q_1}^s, as shown in Ref. [14], $\theta(x)$ is the Heaviside function, $\omega=\mathbf{q}\cdot\mathbf{v}$, and $\omega_1=\mathbf{q}_1\cdot\mathbf{v}$.

We have calculated linear and quadratic contributions to the electronic energy-loss straggling for a wide range of non-relativistic velocities of the projectile, after substitution of the full RPA linear and quadratic response functions into Eqs. (3) and (4). The result of this calculation for an electron density parameter $r_s=2$ ($r_s=[3/4\pi n]^{1/3}$, n being the electron density) and $Z_1=1$ is presented in Fig. 1, as a function of the velocity of the projectile, by dashed (linear contribution) and solid (quadratic contribution) lines, together with the total (linear + quadratic) energy-loss straggling of protons (dashed-dotted line) and antiprotons (dotted line). It is obvious from this figure that at low and intermediate velocities quadratic contributions result in a significant reduction of the energy-loss straggling of antiprotons. On the other hand, though at low velocities the Z_1^3 effect appears to be more important in the energy-loss straggling than in the evaluation of both the stopping power and the energy-width, at high velocities the quadratic contribution to the energy-loss straggling decreases very rapidly.

The numerical results of the total RPA Z_1^3 contribution to the energy-loss straggling for different values of the electron density parameter r_s are illustrated in Fig. 2. At low velocities, the Z_1^3 term gets larger as the electron density increases, as discussed in Ref. [16]. At high velocities, Z_1^3 corrections to both the stopping power and the energy-loss straggling present similar dependences on the electron density.

For completeness, the low-velocity limit of the energy-loss straggling of protons and antiprotons is presented in Fig. 3, as a function of the electron density parameter r_s, as obtained up to third order in the projectile charge after substitution of the low-frequency forms of both linear and quadratic response functions into Eqs. (3) and (4). Since exchange and correlation are absent in our RPA treatment, we have also represented, in the same figure, full nonlinear self-consistent Hartree calculations like the ones presented in Ref. [16]. This figure indicates that in the case of antiprotons with $r_s \lesssim 2$ our quadratic response calculations agree, in the low velocity limit, with the corresponding full nonlinear results; accordingly, our calculations are expected to give, for these electron densities, good account of the full nonlinear energy-loss straggling of antiprotons moving at arbitrary velocities. In the case of protons our quadratic response calculations appear to be accurate, in the low velocity limit, only at high electron densities ($r_s \lesssim 1.5$).

The results depicted in Figs. 1, 2 and 3 indicate that the Z_1^3 contribution to the energy-loss straggling in an electron gas is positive for $Z_1>0$, for all velocities of the projectile and all electron densities of the target. As a result, the energy-loss straggling is, within quadratic response theory, greater for a proton than for an antiproton, as in the case of the stopping power. This result is, at high electron densities, in agreement with full nonlinear self-consistent Hartree calculations, as discussed in Ref. [16]. At low electron densities self-consistent Hartree calculations still predict, in the low-velocity limit, nonlinear effects to reduce the energy-loss straggling of antiprotons. However, the formation around protons of bound states, not described within perturbation theory, tends to screen out interactions with the electron gas, and this causes, at low electron densities, a significant reduction in the energy-loss straggling of protons, as can be inferred from Fig. 3. This reduction can be accounted for through the introduction of an effective charge, as discussed in Refs. [17] and [18].

In summary, we have calculated Z_1^3 corrections to the

energy-loss straggling of protons and antiprotons moving at arbitrary nonrelativistic velocities in a homogeneous electron gas, by using a quadratic response theory and the RPA. At high velocities (after the plasmon threshold), the quadratic response theory provides an accurate estimate of the full nonlinear correction to the energy-loss straggling of protons and anitprotons moving in an electron gas. In the case of antiprotons moving at arbitrary nonrelativistic velocities in many solids used in the experiments ($r_s \lesssim 2$), the present quadratic response theory provides an accurate description of nonlinearities in the energy-loss straggling. A comparison with results obtained within linear response theory indicates that at low and intermediate velocities the Z_1^3 correction reduces significantly the energy-loss straggling of antiprotons, this correction being, at low velocities, more important than in the evaluation of the stopping power.

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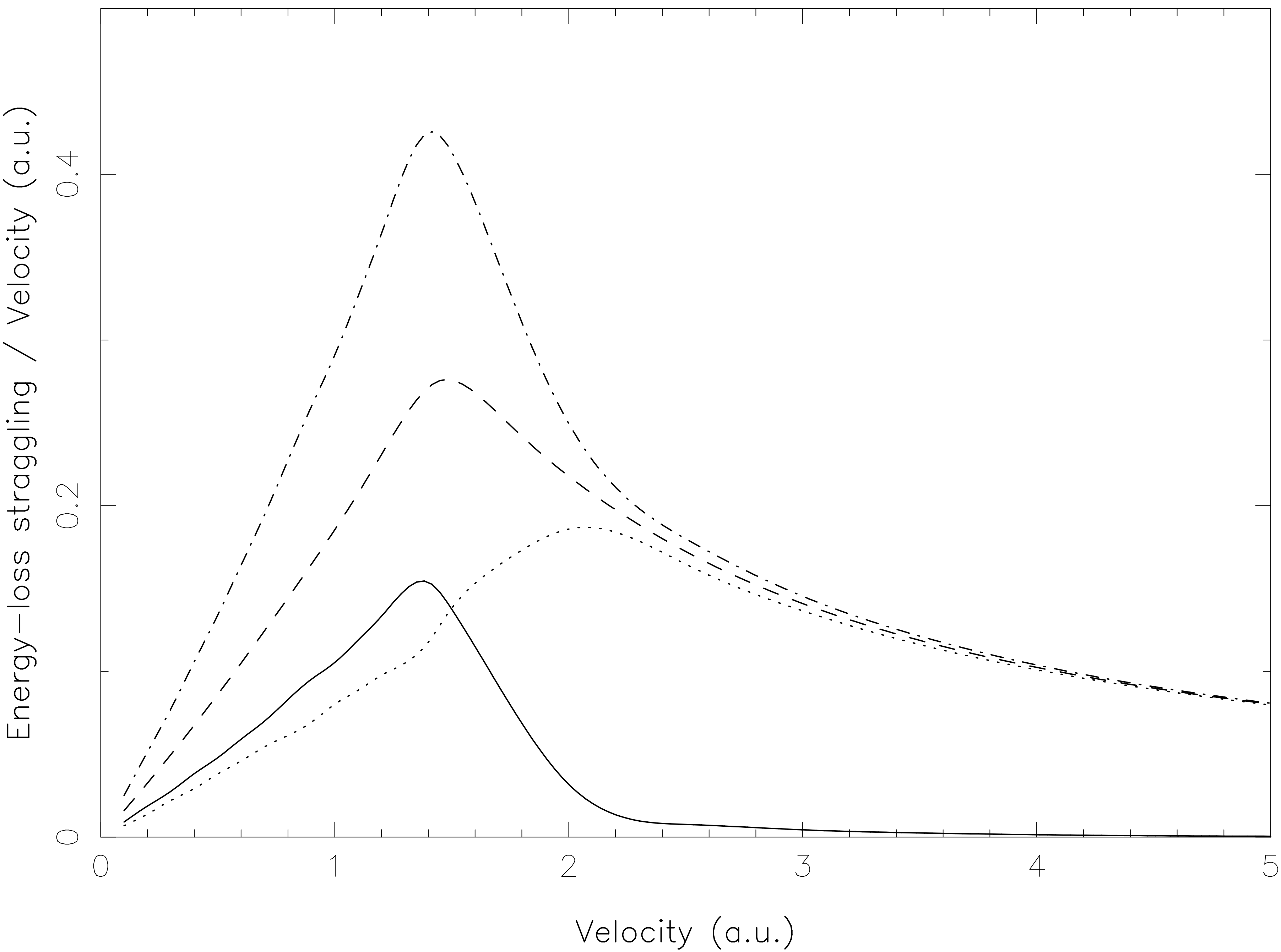
FIG. 1. Linear (dashed line) and quadratic (solid line) contributions to the energy-loss straggling per unit path length for $Z_1 = 1$ and $r_s = 2$, divided by the velocity of the projectile and as a function of the velocity. Total (linear + quadratic) energy-loss stragglings of protons and antiprotons, divided by the velocity, are represented by dashed-dotted and dotted lines, respectively.

FIG. 2. Quadratic (Z_1^3) contribution to the energy-loss straggling per unit path length, divided by the velocity of the projectile and as a function of the velocity, for $Z_1 = 1$ and four representative values of r_s: $r_s = 1$, $r_s = 2$, $r_s = 4$, and $r_s = 6$.

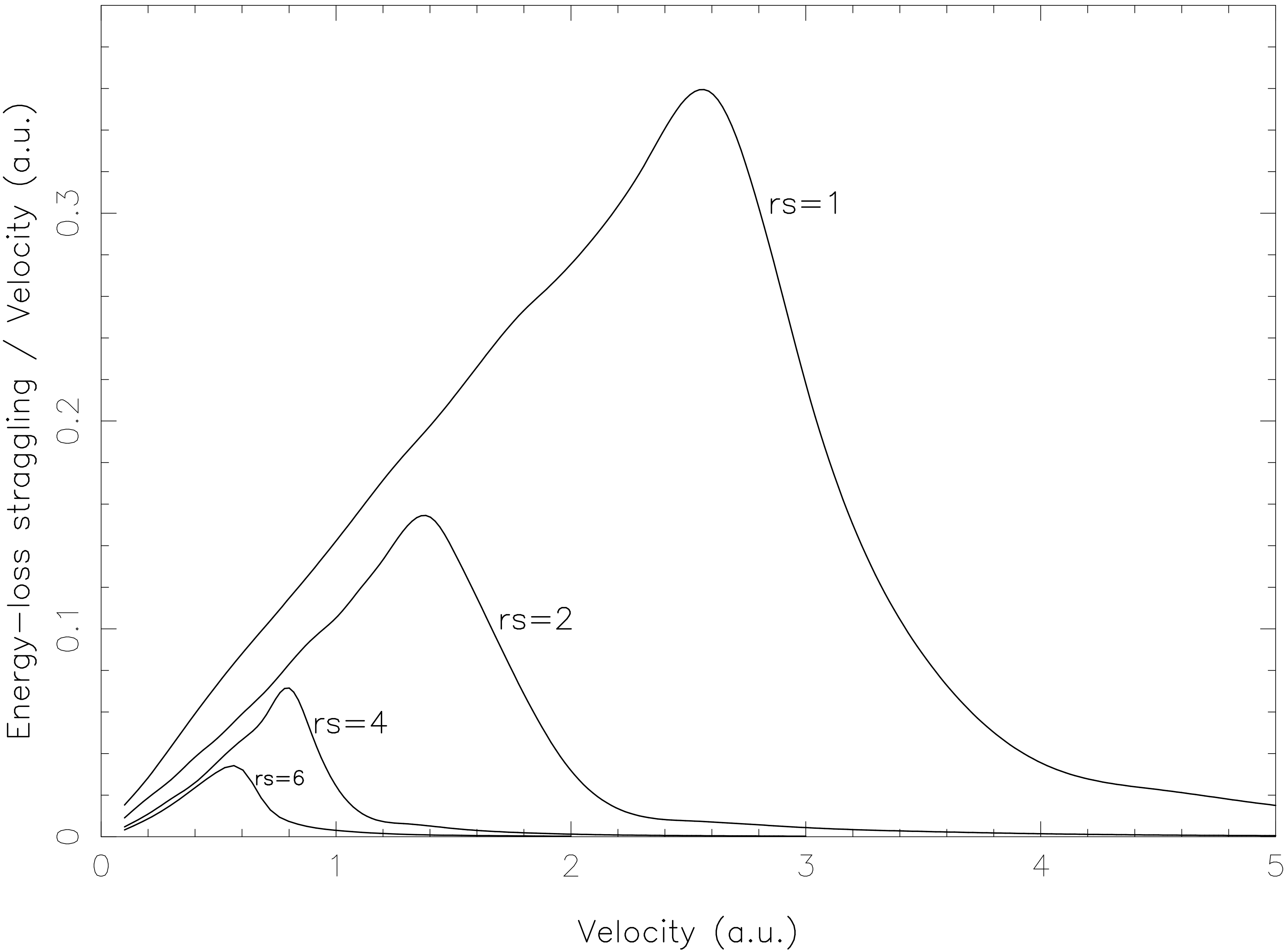
FIG. 3. Total (linear + quadratic) energy-loss straggling per unit path length divided by the square of the projectile velocity, as a function of the electron density parameter r_s, for protons (dashed line) and antiprotons (dashed-dotted line). Crosses and stars represent the full nonlinear energy-loss straggling of protons and antiprotons, respectively. The solid curve represents the linear contribution to the energy-loss straggling for $Z_1 = 1$.

Fig. 1



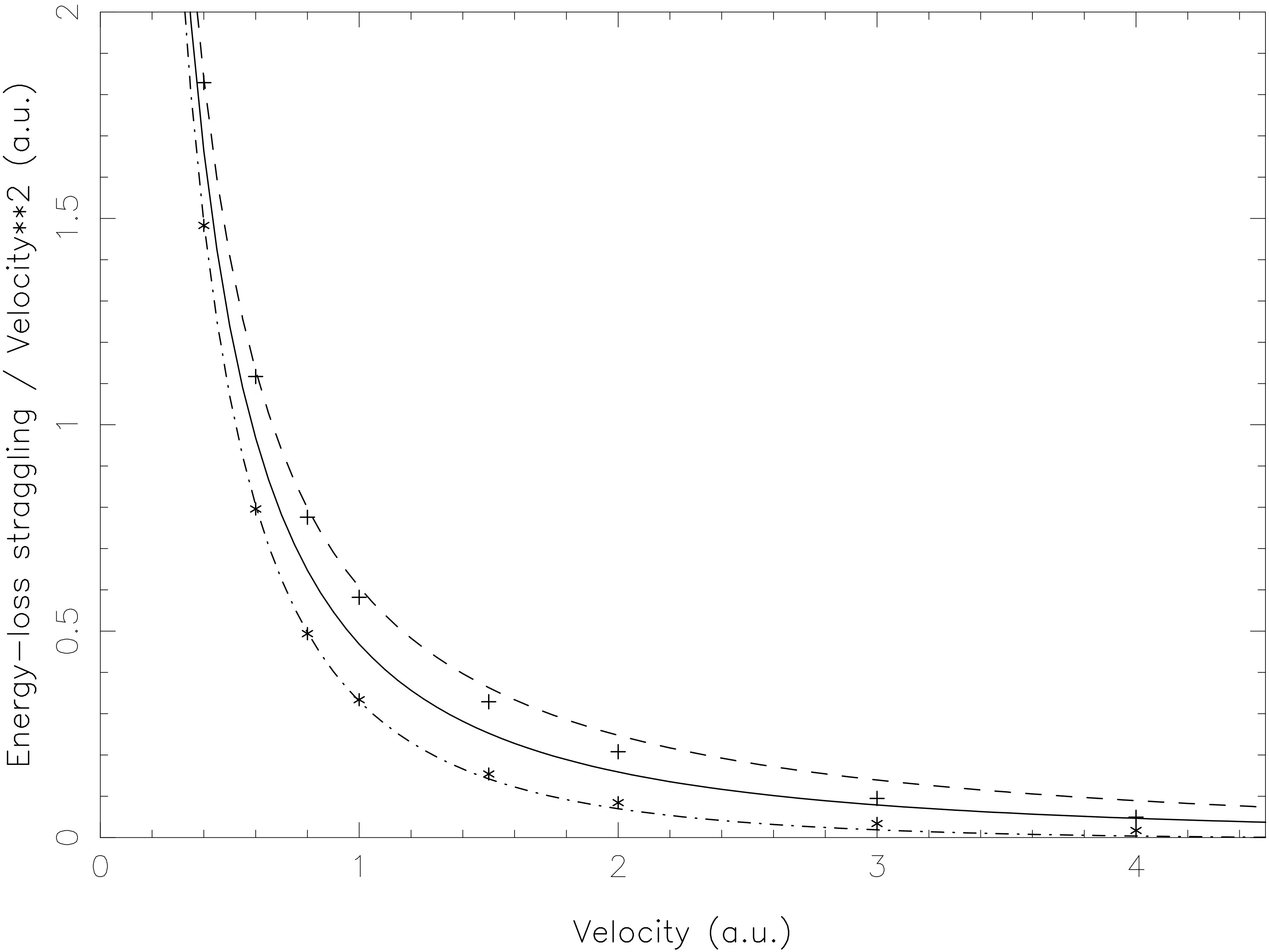
Energy-loss straggling / Velocity (a.u.)
0
0.2
0.4
0
1
2
3
4
5
Velocity (a.u.)

Fig. 2



rs=1
rs=2
rs=4
rs=6
0
0.1
0.2
0.3
Energy-loss straggling / Velocity (a.u.)
0
1
2
3
4
5
Velocity (a.u.)

Fig. 3



Energy-loss straggling / Velocity**2 (a.u.)
Velocity (a.u.)
0
0.5
1
1.5
2
0
1
2
3
4